

An Evaluation of Energy Per Particle (E/N) of Two Dimensional Bose Gas using HD, SD and PP Potential

U. N. SINGH and L. K. MISHRA

Department of Physics,
Magadh University, Bodh-Gaya-824234, Bihar, INDIA
Department of Physics,
Kishori Sinha Mahilla College, Aurangabad, Bihar, INDIA

(Received on : May 31, 2012)

ABSTRACT

In this paper, we have pressed a method of evaluation of energy per particle (E/N) of two dimensional Bose Gas using three potential namely HD (Hard-disc potential), SD (Soft disc potential), PP (Zero-range pseudopotential). By using a zero-range pseudopotential we have estimated $na_{2D}^2 = 0.04$ as the critical density at which the system becomes unstable against cluster formation.

Keywords: many-body correlation, quantum fluctuation, Bose-Einstein Condensate, Critical density, Cluster formation.

1. INTRODUCTION

Degenerate low-dimensional gases are presently attracting considerable interest as model system to investigate beyond mean-field effects and phenomena where many-body correlations and thermal and quantum fluctuation play a relevant role.¹ In two dimensions (2D), it is well known that thermal excitation destroy long-range order and Bose-Einstein Condensate (BEC) cannot exist in large bosonic systems at finite

temperature.² Nevertheless, a defect mediated phase transition from a high temperature normal fluid to a low temperature superfluid was predicted by Berezinski, Kosterlitz and Thouless (BKT)³ and was observed in thin films of liquid ⁴He.

At zero temperature, fluctuations are instead negligible and BEC is possible. The ground-state energy per particle of a homogeneous dilute Bose gas in 2D was first calculated by Schick⁵ and is given by

$$\frac{E_{MF}}{N} = \frac{2\pi\hbar^2}{m} \frac{n}{\ln(1/na_{2D}^2)} \quad (1)$$

Where m is the mass of the particle, n is the number density, and a_{2D} is the 2D scattering length. The above result holds for small values of the gas parameter, $na_{2D}^2 \ll 1$, and can be obtained within a mean-field approximation using the coupling constant

$$g_{2D} = \frac{4\pi\hbar^2}{m} \frac{1}{\ln(1/na_{2D}^2)} \quad (2)$$

The presence at low energy of a density-dependent coupling constant is a peculiar feature of 2D systems.

Bose gases in quasi-2D have been realized with spin-polarized hydrogen on a liquid-helium surface⁶ and with alkali-metal atoms confined in highly anisotropic harmonic traps.⁷⁻⁹ In these systems, the transverse motion of the atoms is frozen to zero-point oscillations resulting in fully 2D kinematics, but the interatomic scattering processes are still 3D. In fact, the 3D s-wave scattering length a_{3D} is always much smaller than the characteristic length of the tight transverse confinement. Theoretical studies of quasi-2D trapped systems predict the existence of a low-temperature quasi condensate phase^{10,11} whose properties have been investigated using mean-field approaches.¹² The nature of the transition in confined systems and whether it belongs to the BEC or BKT universality class is still an open problem both experimentally and theoretically.

An important theoretical prediction for quasi-2D Bose gases in harmonic traps is

the renormalization of the coupling constant due to the tight confinement in one direction. To logarithmic accuracy the result is given by^{11,13}

$$g_{2D} = \frac{2\sqrt{2}\pi\hbar^2}{m} \frac{1}{\frac{a_z}{a_{3D}} + \frac{1}{\sqrt{2\pi}} \ln[1/n(0)a_z^2]} \quad (3)$$

Where $a_z = \sqrt{\hbar/m\omega_z}$ is the oscillator length, fixed by the frequency ω_z of the tight transverse confinement, and $n(0)$ is the 2D density in the center of the trap. If $a_{3D} \ll a_z$, one can neglect the logarithm term in Eq. (3) and the resulting coupling constant is determined by the 3D scattering length. On the contrary, If $a_{3D} \gg a_z$, g_{2D} becomes independent of the value of a_{3D} and a regime of pure 2D scattering is achieved with $a_{2D} = a_z$. This regime is highly interesting and can be realized in trapped gases by using a Feshbach resonance¹⁴ to achieve large value for a_{3D} .

2. MATHEMATICAL FORMULAE USED IN THE EVALUATION

We consider a homogeneous system of N spinless bosons 2D described by the many-body Hamiltonian

$$H = \frac{\hbar^2}{2m} \sum_{i=1}^N \nabla_i^2 + \sum_{i < j} V(r_i - r_j) \quad (4)$$

Where $r_i = x_i \hat{i} + y_i \hat{j}$ denotes the 2D position vector of the i th particle and $V(r)$ is

the two-body interatomic potential. We are different choices for the interatomic potential $V(r)$.

(i) Hard-disk (HD) potential defined by

$$v^{HD}(r) = \begin{cases} \infty & (r < a_{2D}) \\ 0 & (r > a_{2D}) \end{cases} \quad (5)$$

in which case the hard disc diameter corresponds to the scattering length a_{2D} .

(ii) Soft-disk (SD) potential defined by

$$V^{SD}(r) = \begin{cases} V_0 & (r < R) \\ 0 & (r > R) \end{cases} \quad (6)$$

in which case the scattering length is given in terms of the modified Bessel function $I_0(x)$ and its derivative $I'_0(x)$

$$a_{2D} = \text{Re} \exp \left[-\frac{1}{RK_0} \frac{I_0(RK_0)}{I'_0(RK_0)} \right] \quad (7)$$

where $K_0^2 = mV_0 / \hbar^2$ with $V_0 > 0$. For a finite V_0 one has always $R > a_{2D}$; if $V_0 \rightarrow +\infty$, the SD and HD potential coincide with $a_{2D} = R$. In the present calculations, the range of the SD potential is kept fixed to the value $R = 5a_{2D}$ and the height V_0 is determined through Eq. (7) to give the desired value of g_{2D} .

(iii) Zero-range pseudopotential (PP) defined by¹⁵

$$V^{PP}(r) = -\frac{2\pi\hbar^2}{m} \frac{\delta(r)}{\ln(qa_{2D})} \left[1 - \ln(qr) r \frac{\partial}{\partial r} \right] \quad (8)$$

where the second term in the square brackets is a regularizing operator with q an arbitrary wave vector. The potential $V^{PP}(r)$ supports a two-body bound state with energy

$$\epsilon_b = a - 4\hbar^2 / (ma_{2D}^2 e\gamma)$$

And wave function

$$f_b(r) = K_0(2r / (a_{2D} e\gamma)),$$

where $K_0(x)$ is the modified Bessel function and $\gamma \approx 0.577$ is the Euler constant.

The calculations with the repulsive potential $V^{HD}(r)$ and $V^{SD}(r)$ are carried out using the diffusion Monte Carlo (DMC) method. This technique solves the many-body time independent Schrodinger equation by evolving the function

$$f(R, \tau) = \psi_T(R) \Psi(R, \tau)$$

in imaginary time $\tau = it / \hbar$ according to the time dependent Schrodinger equation

$$-\frac{\partial f(R, \tau)}{\partial \tau} = -D \nabla_R^2 f(R, \tau) + D \nabla_R \cdot [F(R) f(R, \tau)] + [E_L(R) - E_{ref}] f(R, \tau) \quad (9)$$

Here $\Psi(R, \tau)$ denotes the wave function of the system and $\psi_T(R)$ is a trial function used for importance sampling used for importance sampling. In the above equation

$$R = (r_1, \dots, r_N), E_L(R) = \psi_T(R)^{-1} H \psi_T(R)$$

Denotes the local energy,

$$F(R) = 2\psi_T(R)^{-1} \nabla_R \psi_T(R)$$

is the quantum drift force, $D = \hbar^2 / (2m)$ plays the role of an effective diffusion constant, E_{ref} is a reference energy introduced to stabilize the numeric. The

energy and other observables of the ground state of the system are calculated from averages over the asymptotic distribution function $f(R, \tau \rightarrow \infty)$. Apart from statistical errors, the DMC method determines the ground-state energy of a system of N bosons exactly.

In the case of the pseudo potential $V^{pp}(r)$ Eq.(8), the gas like state is not the ground state of the system, but is a highly excited state of the Hamiltonian. We expect, however, that for small values of the gas parameter, $na_{2D}^2 \ll 1$, the gas like state is stable against formation of many-body bound states. The calculations with the PP potential are performed at the level of the variational Monte Carlo (VMC) method to avoid the technical difficulties that arise in the study of excited states in the DMC method. Nevertheless, the accuracy achieved by using this variational approach is very high. The VMC technique is based on the variational principle

$$\frac{\langle \psi_T | H | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle} \geq E \quad (10)$$

which is here applied to excited states of the Hamiltonian H . For a trial wave function ψ_T with a given symmetry, the variational estimate provides an upper bound to the energy E of the lowest excited state of the Hamiltonian H with that symmetry.

In all the calculations the trial wave function $\psi_T(R)$ is taken of the Jastrow form

$$\psi_T(r_1, \dots, r_N) = \prod_{i < j} f(r_{ij}) \quad (11)$$

Where the correlation factor $f(r)$ is chosen as the solution of the two-body Schrodinger equation subject to the boundary conditions $f(r \geq d) = 1$ and $f'(r \geq d) = 0$ on the wave function and its first derivative, respectively, with d a variational parameter. For the repulsive potential, HD and SD, $f(r)$ corresponds to the ground-state two-body wave function. On the contrary, in the case of the PP interaction, $f(r)$ is chosen as the two-body wave function corresponding to the lowest excited state with positive energy. The pseudopotential V^{pp} imposes the following boundary condition on the pair wave function for zero inter particle distance:

$$\frac{[rf'(r)]_{r=0}}{[f(r) - \ln(qr)ef']_{r=0}} = -\frac{1}{\ln(qa_{2D})} \quad (12)$$

The free two-particle problem in $2D - \hbar^2 / m \nabla^2 f(r) = \hbar^2 k^2 / m f(r)$, holding $r \neq 0$ gives the general solution

$$F(r) = AJ_0(kr) + BY_0(kr) \quad (13)$$

in terms of the $J_0(x)$ and $Y_0(x)$ Bessel functions. The boundary condition (12) is imposed by the relation

$$a_{2D} = \frac{2e^{-\gamma}}{k} \exp\left(-\frac{\pi A}{2B}\right) \quad (14)$$

In addition we require that $f(r)$ possess only one node for distance $0 < r < d$. The boundary conditions at $r = d$ together with Eq. (14) fix the values of the constant A and B and of the wave vector k . if $d \gg a_{2D}$, the eigen energy $\hbar^2 k^2 / m$ is small and the node of $f(r)$ is located at $r = a_{2D}$.

3. DISCUSSION OF RESULTS

In this paper, we have presented method of evaluation of energy per particle (E/N) as a function of gas parameter Na_{2D}^3

The calculations have been performed for three model potential V^{HP} , V^{SD} and V^{PP} . The results are shown in table T1. The calculations are based on the theoretical

formalism of Mazzanti *et al.*¹⁶ using the hyperfine head chain approach and VMC at high densities by Xing¹⁷ using the VMC method. The DMC results for the HD system are compared with the mean-field results eq.

(1). From the evaluated results we observe that the agreement upto large value of Na_{2D}^3 is quite good.

Table T1

Energy per particle E/N corresponding to the model potential V^{HD} (DMC results), V^{SD} (DMC results) and V^{PP} (VMC results)
[energies are in units of $\hbar^2 / (2Ma_{2D}^2)$]

Na_{2D}^2	HD	SD	PP
1×10^{-7}	$7.738(3) \times 10^{-8}$	$7.732(6) \times 10^{-8}$	
3×10^{-7}	$2.500(1) \times 10^{-7}$	$2.498(1) \times 10^{-7}$	
1×10^{-6}	$9.103(5) \times 10^{-7}$	$0.909(1) \times 10^{-6}$	$9.162(7) \times 10^{-7}$
3×10^{-6}	$2.982(2) \times 10^{-6}$	$2.997(4) \times 10^{-6}$	
1×10^{-5}	$1.108(2) \times 10^{-5}$	$1.106(1) \times 10^{-5}$	$1.115(1) \times 10^{-5}$
3×10^{-5}	$3.710(4) \times 10^{-7}$	$3.702(2) \times 10^{-5}$	
1×10^{-4}	$1.417(1) \times 10^{-4}$	$1.415(1) \times 10^{-4}$	$1.428(1) \times 10^{-4}$
3×10^{-4}	$4.922(5) \times 10^{-4}$	$4.910(2) \times 10^{-4}$	
1×10^{-3}	$1.981(4) \times 10^{-3}$	$1.972(1) \times 10^{-3}$	$1.994(1) \times 10^{-3}$
3×10^{-3}	$7.340(2) \times 10^{-3}$	$7.724(3) \times 10^{-3}$	
1×10^{-2}	$3.296(5) \times 10^{-2}$	$3.057(2) \times 10^{-2}$	$3.304(4) \times 10^{-2}$
3×10^{-2}	$1.436(2) \times 10^{-1}$	$1.105(1) \times 10^{-1}$	$1.369(6) \times 10^{-1}$
1×10^{-1}	$8.940(2) \times 10^{-1}$	$4.161(4) \times 10^{-1}$	

CONCLUSION

We have carried out a study of the ground-state properties of a 2D homogeneous Bose gas with quantum Monte Carlo techniques. The universal behavior of the equation of state for small values of the

gas parameter has been investigated by analyzing both mean-field and beyond mean-field contributions. By using a zero-range pseudopotential to describe interatomic interactions we have estimated $na_{2D}^2 = 0.04$ is the critical density at which

the system becomes unstable against cluster formation. These results are relevant for present and future experiments with ultracold Bose gases in highly anisotropic harmonic traps.

REFERENCES

1. Proceedings of Euroschool on Quantum Gases in Lower Dimensions, Les Houches, edited by L. Pricoupenko, H. Perrin and M. Olshanii, *J. Phys. IV*. (2003).
2. P.C. Hohenberg, *Phys. Rev.* 158, 383 (1967).
3. V.L. Berezinskii, *Zh. Eksp. Teor. Fiz.* 59, 907 (1970) [*Sov. Phys. JETP* 32, 493 (1971)]; J.M. Kosterlitz and D.J. Thouless, *J. Phys. C* 6, 1181 (1973).
4. D.J. Bishop and J.D. Reppy, *Phys. Rev. Lett. (PRL)* 40, 1727 (1978).
5. M. Schick, *Phys. Rev. A* 3, 1067 (1971).
6. A. I. Safonov, D. S. Petrov, B. P. Vanzyl and N. L. Smith., *Phys. Rev. Lett. (PRL)* 81, 4545 (1998).
7. A. Gorlitz, S. Berger, C. H. Schuneck, Y. Shin and W. Ketterle., *Phys. Rev. Lett. (PRL)* 87, 130402 (2001)
8. D. Rychtarik, B. Emgeser, H.C. Nagerl and R. Grimm, *Phys. Rev. Lett. (PRL)* 92, 173003 (2004).
9. N.L. Smith, J. D. Reddy, M. E. Gehm, J. E. Thomas and D. S. Jin, e-print cond-mat/0410101 (2005).
10. V.N. Popov in *Functional Integrals in Quantum Field Theory and Statistical Physics*, Reidel, Dordrecht, (1983).
11. D.S. Petrov, M. Holzmann and G.V. Shlyapnikov, *Phys. Rev. Lett. (PRL)* 84, 2551 (2000).
12. C. Gies, B.P. van Zyl, S.A. Morgan and D.A.W. Hutchinson, *Phys. Rev. A* 69, 023616 (2004); L. Pricoupenko, *Phys. Rev. A* 70, 013601 (2004).
13. D.S. Petrov and G.V. Shlyapnikov, *Phys. Rev. A* 64, 012706 (2001).
14. T. Lofros, M. Veilleite, E. G. Moon, J. Carbon and S. Reddy., *Phys. Rev. Lett. (PRL)* 88, 173201 (2002).
15. M. Olshanii and L. Pricoupenko, *Phys. Rev. Lett. (PRL)* 88, 010402 (2002).
16. F. Mazzanti, A. Polls and A. Fabrocini, e-print cond-mat/0410690. (2002)
17. Lei Xing, *Phys. Rev. B.* 42, 8426 (1990).
18. S. Giorgini, J. Boronat and J. Casulleras, *Phys. Rev. A* 60, 5129 (1999).
19. D.F. Hines, N.E. Frankel and D.J. Mitchell, *Phys. Rev. A* 68, 12 (1978); E.B. Kolomeisky and J.P. Straley, *Phys. Rev. B* 46, 11749 (1992); A. A. Ovchinnikov, *J. Phys.: Condens. Matter* 5, 8665 (1993); J.O. Anderson, *Eur. Phys. J. B.* 28, 389 (2002).
20. J. Boronat and J. Casulleras, *Phys. Rev. B* 49, 8920 (1994).
21. R. Combescot, A. Recati, G. Lobo, F. Chevy and M. M. Parish., *Phys. Rev. Lett. (PRL)* 100, 180402 (2007).
22. P. Massighan, G. M. Run, H.T. F. Stoof, W. Ketterle and R. G. Hublet, *Phys. Rev. A* 78, 031602 (2008).